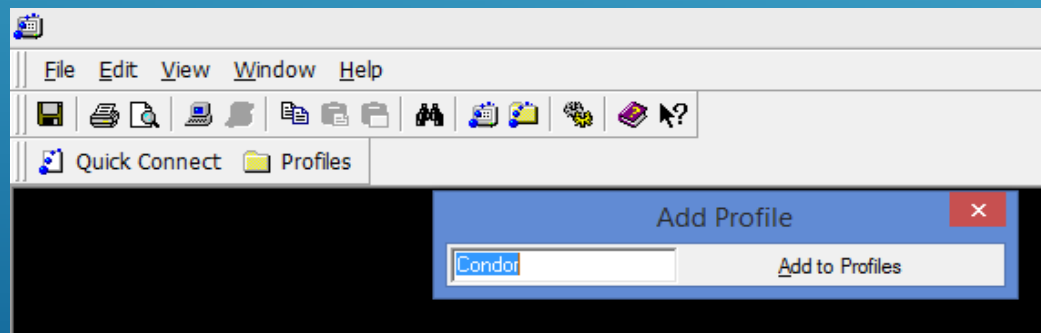
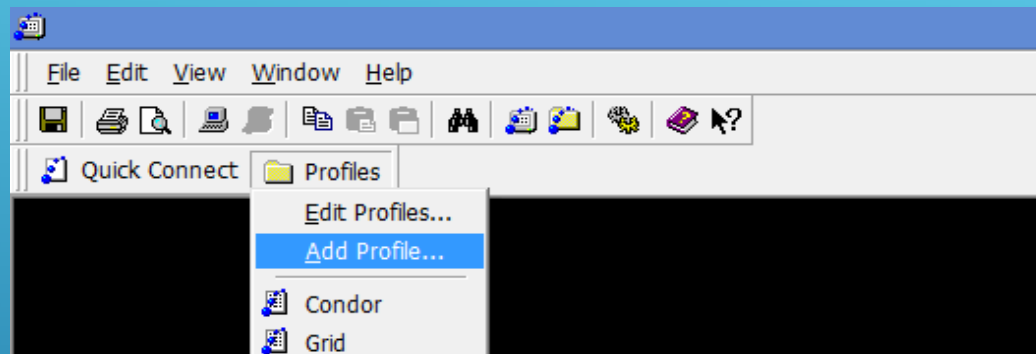
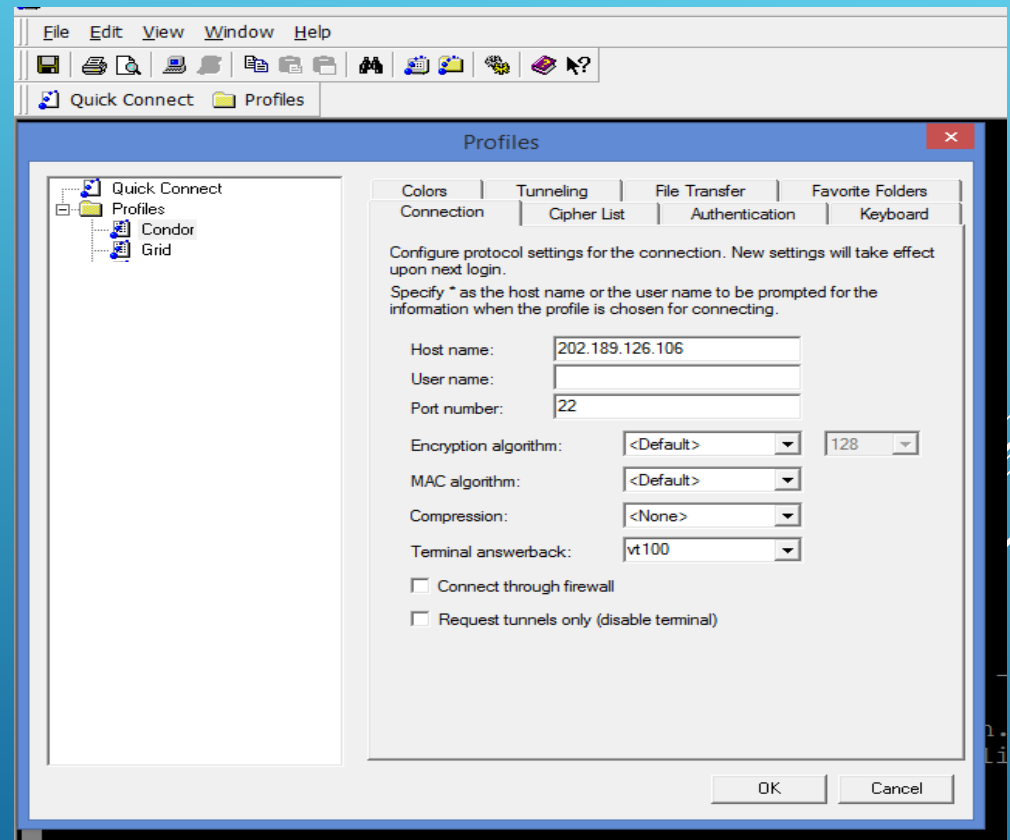
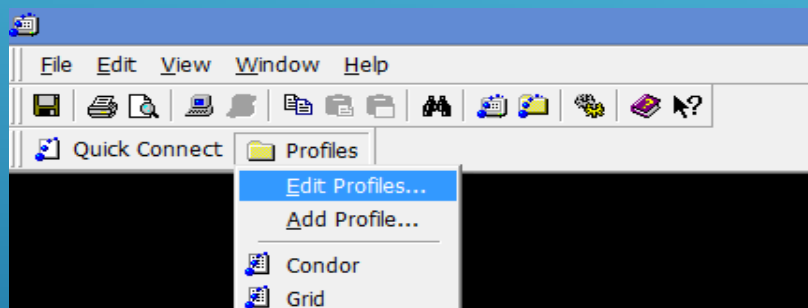


# Setup the Condor Profile in SSh



# Edit the Condor Profile in SSh



# Edit the firefly.con in Condor account

7z.dll 7z.exe 7zip.dll ff.7z firefly.bat firefly.con Test-RHF.inp

List of the PCGAMESS files in your account, you just need to modify few lines in the "firefly.con"

```
File Edit View Window Help
Quick Connect Profiles
Executable = firefly.bat
#arguments = $(Process)

request_cpus = 4

#Lab's PC
Requirements = OpSys == "WINDOWS" && ( Arch == "INTEL" || Arch == "AMD64" )

#Any PC
#Requirements = OpSys == "LINUX" && Arch == "INTEL"

TRANSFER_FILES = ALWAYS
should_transfer_files = YES
when_to_transfer_output = ON_EXIT_OR_EVICT

transfer_input_files = 7z.exe, 7z.dll, 7zip.dll, ff.7z, firefly.bat, \
Test-RHF.inp

#transfer_output_files = OUTPUT_vina.pdbqt

#Input = Test-RHF.inp
Output = Test-RHF.out
#Rank = kfiops

arguments = Test-RHF.inp
#transfer_output_files = EXAM$(Process).out
Queue

#arguments = EXAM$(Process)
#transfer_output_files = EXAM$(Process).out
#Queue 22
```

PCGAMESS input file name:  
Test-RHF.inp

PCGAMESS output file name:  
Test-RHF.out

# Input file and Run command

```
File Edit View Window Help
[Icons]
Quick Connect Profiles

$CONTRL RUNTYP=OPTIMIZE UNITS=ANGS $END
$SYSTEM TIMLIM=600000000000000000000000000000 MWORDS=250 $END
$SCF DIRSCF=.True. $END
$GUESS GUESS=HUCKEL $END
$BASIS GBASIS=N311 NGAUSS=6 NDFUNC=1 NPFUNC=1 DIFFSP=.T. DIFFS=.T. $END
$STATPT NSTEP=200 $END
$DATA
Si3C6H14 RHF/6-311++G(d,p)
C1
SILICON      14.0    -0.469805961    -0.935439370    0.848660773
CARBON       6.0     -1.085557859    -2.578722309    1.465794171
CARBON       6.0     -1.910100737    -1.975057136    0.296276209
HYDROGEN     1.0     0.741352896    -0.890327127    0.018045297
HYDROGEN     1.0     -0.517339246    -3.475961749    1.235587508
HYDROGEN     1.0     -1.848439378    -2.501435362   -0.652422876
HYDROGEN     1.0     -2.918694969    -1.652456431    0.540351141
CARBON       6.0     -0.789245980    0.591280345    1.861915423
SILICON      14.0    -1.527407287    0.436832702    3.168134423
CARBON       6.0     -0.051084673    0.745727989    3.168134423
HYDROGEN     1.0     -0.975725270    1.482532509    1.270408423
HYDROGEN     1.0     -1.842330260   -0.559329320    3.463888423
HYDROGEN     1.0     -2.215288839    1.223175008    3.463888423
HYDROGEN     1.0     0.263838300    1.741890010    3.463888423
HYDROGEN     1.0     0.636796880   -0.040614317    3.463888423
CARBON       6.0     -1.797014998    -2.647114250    2.829887747
CARBON       6.0     -1.553881574    -3.855284166    3.699459974
SILICON      14.0    -2.885311370    -3.675039334    3.014075953
HYDROGEN     1.0     -1.915920746    -1.682744312    3.314488120
HYDROGEN     1.0     -1.507637155    -3.711574452    4.774724896
HYDROGEN     1.0     -0.887102855    -4.627723143    3.328340252
HYDROGEN     1.0     -3.122917514    -4.325045496    2.177403382
HYDROGEN     1.0     -3.743451814    -3.408896805    3.623788026
$END
```

Run command:

condor\_submit firefly.con